2007 FEB 28

201-16554P

I U C L I D

Data Set

Existing Chemical	:	ID: 111381-89-6
Memo	:	HPV Chemical
CAS No.	:	111381-89-6
TSCA Name	:	1,2-Benzenedicarboxylic acid, heptyl nonyl ester, branched and linear
Synonym	:	1,2-benzenedicarboxylic acid (C7-C9) ester, branched and linear
Producer related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Substance related part		
Company	:	ExxonMobil Biomedical Sciences Inc.
Creation date	:	18.10.2000
Status	:	
Memo	:	ACC Phthalate Ester Panel HPV Testing Group
Printing date	:	05.07.2006
Revision date	:	
Date of last update	:	05.07.2006
Number of pages	:	23
Chapter (profile)	:	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile)	:	Reliability: without reliability, 1, 2, 3, 4
Flags (profile)	:	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	lead organisation
Name	:	ACC Phthalate Esters Panel HPV Testing Group
Contact person	:	Dr. Marian Stanley
Date	:	
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Town	:	22209 Arlington, VA
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Homepage	:	

Remark : The American Chemistry Council Phthalate Esters Panel includes the following member companies:

BASF Corporation
CONDEA Vista Company
Eastman Chemical Company
ExxonMobil Chemical Company
Ferro Corporation
ICI Americas / Uniqema
Sunoco Chemicals
Teknor Apex Company

02.11.2001

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is part of the Transitional Phthalate Esters subcategory. The subcategory includes the following six CAS numbers: 68515-50-4, 71888-89-6, 27554-26-3, 68515-44-6, 111381-89-6 and 111381-90-9 (see remark for names)

Remark : This chemical is part of the Transitional Phthalate Esters subcategory. The subcategory includes the following six CAS numbers and names:

68515-50-4 1,2,-benzenedicarboxylic acid, dihexyl ester, branched and linear (DHP)

71888-89-6 1,2-benzenedicarboxylic acid, di C6-8 branched alkyl ester, C7 rich (DIHP)

27554-26-3 1,2,-benzenedicarboxylic acid, diisooctyl ester (DIOP)

68515-44-6 1,2-benzenedicarboxylic acid, diheptyl ester, branched and linear (DinHP)

111381-89-6 1,2-benzenedicarboxylic acid (C7, C9) ester, branched and linear (79P)

111381-90-9 1,2-benzenedicarboxylic acid, (C7,C11) ester, branched and linear (711P)

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250oC) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates are insoluble.

The phthalate esters were subdivided into three subcategories based on their physicochemical and toxicological properties. The phthalate esters in this subcategory, Transitional phthalates, are produced from alcohols with straight-chain carbon backbones of C4-6. Phthalate esters containing >10% C4-6 molecules were conservatively included in this subcategory. Six of the U.S. HPV chemicals, dihexyl (DHP), diheptyl, diisoheptyl, diisooctyl, heptyl nonyl (C7, C9) and heptyl undecyl (C7, C11) phthalates are included in this subcategory. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including dibutyl (DBP), butylbenzyl (BBP), and di(2-ethylhexyl) phthalate (DEHP). Data on a structurally similar material, di-n hexyl phthalate, was also included for read-across purposes.

Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP). Physicochemical properties also vary in that the lower molecular weight transitional phthalates are more water-soluble than higher transitional phthalates, but none would be considered to fall into the "high water soluble" category. What distinguishes these phthalates from others is their greater mammalian toxicity potential, particularly with regard to reproductive and developmental effects, compared to either the low or high molecular weight phthalate subcategories. Of the phthalates in this subcategory, DEHP appears to be the most potent for liver and reproductive/developmental endpoints.

03.04.2006

1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

Purity type	:	
Substance type	:	organic
Physical status	:	liquid
Purity	:	
Colour	:	
Odour	:	

02.11.2001

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use	:	industrial
Category	:	Polymers industry
Remark	:	Transitional phthalates have varied uses from solvents (e.g., dibutyl) to plasticizers for PVC (e.g., DEHP).

02.11.2001

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2.1 MELTING POINT

Value	:	-45 °C
Decomposition	:	no, at °C
Sublimation	:	
Method	:	other: no data
Year	:	
GLP	:	
Test substance	:	other TS: CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear
Remark	:	Data are from a peer reviewed literature review of data from a variety of sources including manufacturer's data or handbook values.
Test substance	:	CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear
Reliability	:	(2) valid with restrictions This robust summary is assigned a reliability of 2 because there is limited informtion on how the data were developed.
Flag	:	Critical study for SIDS endpoint

05.07.2006 (2)

Value	:	64 °C
Decomposition	:	no, at °C
Sublimation	:	no
Method	:	other: calculation
Year	:	
GLP	:	
Test substance	:	other TS: CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear
Method	:	Melting point calculation by MPBPWIN ver. 1.41 using calculation methods of Joback and Gold and Ogle.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation. However, the melting point calculation in EPI SuiteTM gives erroneously high results for the phthalate esters.
Test substance	:	CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear
Reliability	:	(3) invalid

17.04.2006 (3)

2.2 BOILING POINT

Value	:	417 °C at 1013 hPa
Decomposition	:	no
Method	:	other
Year	:	
GLP	:	
Test substance	:	other TS: CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear
Method	:	Boiling point calculation by MPBPWIN ver. 1.41 using calculation method of Stein and Brown.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear
Reliability	:	(2) valid with restrictions

This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint
17.04.2006 (3)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : .000000252 hPa at 25 °C
Decomposition : no
Method : other (calculated)
Year :
GLP :
Test substance : other TS: CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear

Method : Measured data collected and tabulated, calculated data also considered in determining recommended values.

Remark : Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for vapour pressure, represent the definitive and currently accepted physicochemical database for selected phthalate esters including a diisooctyl phthalate, which provides an intermediate value for a heptyl, nonyl phthalate ester.

Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for a diisooctyl phthalate ester was 520.4 cm3 mol-1.

Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water)
r2 = 0.98, SE = 0.39

Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air)
r2 = 0.87, SE = 0.33

Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol)
r2 = 0.19, SE = 0.41

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

Test substance : CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear

Reliability : (2) valid with restrictions
The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
17.04.2006 (1)

Value	:	.00000185 hPa at 25 °C
Decomposition	:	no
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear
Method	:	Vapor pressure calculation by MPBPWIN ver. 1.41 using calculation method of Grain.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.

17.04.2006 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient	:	octanol-water
Log pow	:	7.73 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear
Method	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Remark	:	Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for partition coefficient, represent the definitive and currently accepted physicochemical database for selected phthalate esters including diisooctyl phthalate, which provides an intermediate value for a heptyl, nonyl phthalate ester. Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for a diisooctyl phthalate ester was 520.4 cm3 mol-1. Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water) r2 = 0.98, SE = 0.39 Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air) r2 = 0.87, SE = 0.33 Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol) r2 = 0.19, SE = 0.41 It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths

from 1 to 13 carbons.

Test substance	:	CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear
Reliability	:	(2) valid with restrictions The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
Flag	:	Critical study for SIDS endpoint

17.04.2006 (1)

Partition coefficient	:	octanol-water
Log pow	:	8.39 at 25 °C
pH value	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear
Method	:	Partition coefficient by LOGKOWWIN ver. 1.67 using an atom/fragment calculation method of Meylan and Howard.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.

17.04.2006 (3)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in	:	Water
Value	:	.00249 mg/l at 25 °C
pH value	:	
concentration	:	at °C
Temperature effects	:	
Examine different pol.	:	
pKa	:	at 25 °C
Description	:	
Stable	:	
Deg. product	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear
Method	:	Measured data collected and tabulated, calculated data also considered in determining recommended values.
Remark	:	Physicochemical data for selected commercial phthalate esters from various sources including the public literature, manufacturing secifications, and handbook values were evaluated by an industry peer review process. Valid values were identified and presented in a phthalate ester environmental fate, peer reviewed publication. These data, including the values for water solubility, represent the definitive and currently accepted physicochemical database for selected phthalate esters including diisooctyl phthalate, which provides an intermediate value for a heptyl, nonyl phthalate ester.

Quantitative structure-property relationships, significant at the 99.9% level, were developed using the relevant phthalate ester data to estimate solubility in water, air, and octanol, where V = the Le Bas molar volume (cm3 mol-1). The Le Bas molar volume used for a diisooctyl phthalate ester was 520.4 cm3 mol-1.

Log CS(WL) = -0.012V + 5.8, n = 35 (solubility in water)
r2 = 0.98, SE = 0.39

Log CS(AL) = -0.013V - 1.3, n = 15 (solubility in air)
r2 = 0.87, SE = 0.33

Log CS(OL) = -0.016V + 3.4, n = 68 (solubility in octanol)
r2 = 0.19, SE = 0.41

It was recommended by the authors that the above regressions be used for predicting the three solubilities for phthalate esters with alkyl chain lengths from 1 to 13 carbons.

Test substance : CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear

Reliability : (2) valid with restrictions
The value was calculated based on the QSPR (quantitative structure-property relationship) three-solubility model. This robust summary has a reliability rating of 2 because the data are calculated and not measured.

Flag : Critical study for SIDS endpoint
17.04.2006 (1)

Solubility in : Water
Value : .00024 mg/l at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: calculcated
Year :
GLP :
Test substance : other TS: CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear

Method : Water solubility calculated using WSKOWN ver 1.41 based on Kow correlation method of Meylan and Howard. Kow used in calculation was 8.39.

Remark : EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.

Test substance : CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

17.04.2006 (3)

2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	1 based on intensity of sunlight
Conc. of substance	:	at 25 °C
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	1500000 molecule/cm³
Rate constant	:	.000000000022 cm³/(molecule*sec)
Degradation	:	50 % after 5.9 hour(s)
Deg. product	:	not measured
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear
Method	:	Photodegradation rate calculated by AOPWIN ver. 1.91 based on the methods of Atkinson.
Remark	:	50% degradation after 5.85 hrs or 0.487 days based on a 12-hour day. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPI SuiteTM, 2000) calculates a chemical half-life for a 12-hour day (the 12-hour day half-life value normalizes degradation to a standard day light period during which hydroxyl radicals needed for degradation are generated), based on an OH- reaction rate constant and a defined OH- concentration. EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear
Reliability	:	(2) valid with restrictions This robust summary has a reliability rating of 2 because the data are calculated.
Flag 12.05.2006	:	Critical study for SIDS endpoint (3)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	4.2 year at 25 °C
t1/2 pH9	:	- at °C
Deg. product	:	
Method	:	other (calculated)
Year	:	
GLP	:	
Test substance	:	other TS: CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear
Method	:	Hydrolysis rate calculated by HYDROWIN ver. 1.67 based on work for EPA by T. Mill et al.
Remark	:	EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance	:	CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester,

branched and linear

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint
05.07.2006 (3)

3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year :

Remark : Physicochemical data used in the calculation:

Parameter	Value w/ Units
Molecular Weight	390.57
Temperature	25° C
Log Kow	7.73
Water Solubility	0.00249 g/m3
Vapor Pressure	0.0000252 Pa
Melting Point	-45°C

Result : Using the Mackay Level I calculation, the following distribution is predicted for 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear:

% Distribution	Compartment
0.0	Air
0.0	Water
97.7	Soil
2.2	Sediment
0.1	Suspended Sediment
0.0	Biota

Test substance : CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint
17.04.2006 (4)

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level III
Year :

Remark : Physicochemical data used in the calculation:

Parameter	Value w/ Units
Molecular Weight	390.57
Temperature	25° C
Log Kow	7.73
Water Solubility	0.00249 g/m3
Vapor Pressure	0.0000252 Pa
Melting Point	-45°C

Emissions rates used in the calculation:

Compartment	Rate (kg/hr)
Air	1000
Water	1000
Soil	1000

Half-lives used in the calculation:

Compartment	Half-life (hr)
Air	11.7a
Water	120b
Soil	420c
Sediment	420c

a - as calculated using AOPWIN version 1.91, a subroutine of the computer program EPI SuiteTM version 3.12 and normalized to a 24 hour day [Environmental Protection Agency (EPA) (2000). EPI SuiteTM, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.]

b - based on read-across biodegradation data from two phthalate esters: 1,2-benzenedicarboxylic acid, di-C7 alkyl esters (CAS No. 71888-89-6); Exxon Biomedical Sciences, Inc. (1995). Ready Biodegradability, Manometric Respirometry. Study No. 199894A. Unpublished report. 1,2-benzenedicarboxylic acid, diiso-C9 alkyl esters (CAS No. 68515-48-0); Exxon Biomedical Sciences, Inc. (1995). Ready Biodegradability, Manometric Respirometry. Study No. 199894A. Unpublished report.

Boethling R (2000). HPVC-Screening Tool: Using Ready and Inherent Biodegradability Data to Derive Input Data for the EQC Model, Appendix 10 in Environment Canada, Environmental Categorization for Persistence Bioaccumulation and Inherent Toxicity of Substances on the Domestic Substance List Using QSARs, Results of an international workshop hosted by Chemicals Evaluation Division of Environment Canada, Nov. 11-12, 1999, in Philadelphia, PA, USA.

c - based on Boethling, R. recommendation that half-lives of 3 to 4 times longer than surface water should be used for soil and sediment.

Result : Using the Mackay Level III calculation, the following distribution is predicted for 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear:

Compartment	% Distribution
Air	1.0
Water	8.4
Soil	68.4
Sediment	22.2

Test substance : CAS #111381-89-6; 1,2-benzenedicarboxylic acid, heptyl nonyl ester, branched and linear

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.

Flag : Critical study for SIDS endpoint
12.05.2006 (4)

3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS

4.6.2 TOXICITY TO TERRESTRIAL PLANTS

4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS

4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES

4.7 BIOLOGICAL EFFECTS MONITORING

4.8 BIOTRANSFORMATION AND KINETICS

4.9 ADDITIONAL REMARKS

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.2.1 SKIN IRRITATION

5.2.2 EYE IRRITATION

5.3 SENSITIZATION

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY 'IN VITRO'

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

(1) Cousins I and Mackay D (2000). Correlating the physical-chemical properties of phthalate esters using the 'three solubility' approach. Chemosphere 41, 1389-1399.

(2) David R, McKee R, Butala J, Barter R and Kayser M (2001). Esters of Aromatic Mono, Di and Tricarboxylic acids and Di, Tri, or Polyalcohols. Patty's Industrial Hygiene and Toxicology, Chapter 81, unpublished draft.

(3) Environmental Protection Agency (EPA) (2000). EPI SuiteTM, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

Memo : This chemical is part of the Transitional Phthalate Esters subcategory. Data from other chemicals in this subcategory can be used to assess the potential hazards of all category members.

Remark : Chapters 2, 3, 4 & 5

There are measured physicochemical property data available for some of the transitional phthalates. Computer estimation models were also used to calculate physicochemical and fate data for phthalates in this category. The calculated data were developed from a computer model used by the EPA, as cited in an EPA guidance document prepared for the HPV Challenge Program. Depending upon the endpoint, the modeled data agree with measured data. The combination of measured values and calculated values is sufficient to provide the required information on the physiochemical and fate properties of the HPV phthalates in the transitional group.

A complete health effects SIDS data set is available for dibutyl, butyl benzyl and diethylhexyl phthalate. All of these substances are under review in Europe as part of the Existing Substances Risk Assessment, and have been included as reference compounds in the transitional phthalate subcategory. Data on di-n hexyl phthalate (non-HPV chemical) was also included to support read-across to dihexyl, diheptyl, and diisoheptyl phthalates. The available health effects data on other HPV chemicals in this subcategory are consistent with that reported for the above reference phthalates. Thus, studies from the reference compounds (DBP, BBP, DEHP and di-n hexyl) will be used as read-across to predict the toxicity of the remaining untested members.

There is a full data set for environmental toxicity data on DBP, BBP, DHP, DEHP, and DIOP. The lower transitional phthalates (DBP, BBP) are more water soluble than higher transitional phthalates and cause acute aquatic toxicity in the 1-10 mg/L range. There is an apparent cut-off in acute toxicity at dihexyl phthalate and higher; these results are further confirmed with QSAR modeling. Both calculated and measured values for environmental toxicity endpoints predict no effects at the limit of water solubility. The dihexyl phthalate data, together with read across from DIOP to diheptyl and diisoheptyl provide sufficient test data to indicate that these phthalates have no associated acute aquatic toxicity but may show chronic toxicity. Read across from DEHP, together with QSAR modeling also confirm that diisooctyl phthalate has neither acute nor chronic aquatic toxicity.

05.07.2006

10.3 RISK ASSESSMENT